# QikProp Descriptors and Properties

For each successfully processed molecule, QikProp produces the following descriptors and properties. Those that are not predicted in fast mode are marked with a dagger (†). Those whose values differ between fast and normal mode are marked with a double dagger (‡). Additional information on many of these properties can be found in the *QikProp User Manual*.

*Table 2.1. QikProp properties and descriptors. Range is for 95% of known drugs.*

| Property or Descriptor | Description | Range or recommended values |
|---|---|---|
| **molecule name** | Molecule name taken from the title line in the input structure file. If the title line is blank, the input file name is used. | |
| **#stars** | Number of property or descriptor values that fall outside the 95% range of similar values for known drugs. Outlying descriptors and predicted properties are denoted with asterisks (*) in the `.out` file. A large number of stars suggests that a molecule is less drug-like than molecules with few stars. The following properties and descriptors are included in the determination of #stars: MW, dipole, IP, EA, SASA, FOSA, FISA, PISA, WPSA, PSA, volume, #rotor, donorHB, accptHB, glob, QPpolrz, QPlogPC16, QPlogPoct, QPlogPw, QPlogPo/w, logS, QPLogKhsa, QPlogBB, #metabol | 0 – 5 |
| **#amine** | Number of non-conjugated amine groups. | 0 – 1 |
| **#amidine** | Number of amidine and guanidine groups. | 0 |
| **#acid** | Number of carboxylic acid groups. | 0 – 1 |
| **#amide** | Number of non-conjugated amide groups. | 0 – 1 |
| **#rotor** | Number of non-trivial (not CX3), non-hindered (not alkene, amide, small ring) rotatable bonds. | 0 – 15 |
| **#rtvFG** | Number of reactive functional groups; the specific groups are listed in the *jobname* `.out` file. The presence of these groups can lead to false positives in HTS assays and to decomposition, reactivity, or toxicity problems *in vivo*. See Appendix A of the *QikProp User Manual* for a complete list. | 0 – 2 |
| **CNS** | Predicted central nervous system activity on a –2 (inactive) to +2 (active) scale. | –2 to +2 |
| **mol_MW** | Molecular weight of the molecule. | 130.0 – 725.0 |
| **dipole†** | Computed dipole moment of the molecule. | 1.0 – 12.5 |
| **SASA** | Total solvent accessible surface area (SASA) in square angstroms using a probe with a 1.4 Å radius. | 300.0 – 1000.0 |
| **FOSA** | Hydrophobic component of the SASA (saturated carbon and attached hydrogen). | 0.0 – 750.0 |
| **FISA** | Hydrophilic component of the SASA (SASA on N, O, H on heteroatoms, and carbonyl C). | 7.0 – 330.0 |
| **PISA** | π (carbon and attached hydrogen) component of the SASA. | 0.0 – 450.0 |
| **WPSA** | Weakly polar component of the SASA (halogens, P, and S). | 0.0 – 175.0 |
| **volume** | Total solvent-accessible volume in cubic angstroms using a probe with a 1.4 Å radius. | 500.0 – 2000.0 |
| **donorHB** | Estimated number of hydrogen bonds that would be donated by the solute to water molecules in an aqueous solution. Values are averages taken over a number of configurations, so they can be non-integer. | 0.0 – 6.0 |
| **accptHB** | Estimated number of hydrogen bonds that would be accepted by the solute from water molecules in an aqueous solution. Values are averages taken over a number of configurations, so they can be non-integer. | 2.0 – 20.0 |

*Table 2.1. QikProp properties and descriptors. Range is for 95% of known drugs. (Continued)*

| Property or Descriptor | Description | Range or recommended values |
|---|---|---|
| **dip^2/V†** | Square of the dipole moment divided by the molecular volume. This is the key term in the Kirkwood-Onsager equation for the free energy of solvation of a dipole with volume V. | 0.0 – 0.13 |
| **ACxDN^.5/SA** | Index of cohesive interaction in solids. This term represents the relationship $(accptHB(\sqrt{donorHB}))/(SA)$ ; see *Bioorg. Med. Chem. Lett.* **2000**, *10*, 1155. | 0.0 – 0.05 |
| **glob** | Globularity descriptor, $(4\pi r^2)/(SASA)$ , where *r* is the radius of a sphere with a volume equal to the molecular volume. Globularity is 1.0 for a spherical molecule. | 0.75 – 0.95 |
| **QPpolrz** | Predicted polarizability in cubic angstroms. | 13.0 – 70.0 |
| **QPlogPC16** | Predicted hexadecane/gas partition coefficient. | 4.0 – 18.0 |
| **QPlogPoct‡** | Predicted octanol/gas partition coefficient. | 8.0 – 35.0 |
| **QPlogPw** | Predicted water/gas partition coefficient. | 4.0 – 45.0 |
| **QPlogPo/w** | Predicted octanol/water partition coefficient. | –2.0 – 6.5 |
| **QPlogS** | Predicted aqueous solubility, log S. S in mol $dm^{-3}$ is the concentration of the solute in a saturated solution that is in equilibrium with the crystalline solid. | –6.5 – 0.5 |
| **CIQPlogS** | Conformation-independent predicted aqueous solubility, log S. S in mol $dm^{-3}$ is the concentration of the solute in a saturated solution that is in equilibrium with the crystalline solid. | –6.5 – 0.5 |
| **QPlogHERG** | Predicted $IC_{50}$ value for blockage of HERG $K^+$ channels. | concern below –5 |
| **QPPCaco** | Predicted apparent Caco-2 cell permeability in nm/sec. Caco-2 cells are a model for the gut-blood barrier. QikProp predictions are for non-active transport. | <25 poor, >500 great |
| **QPlogBB** | Predicted brain/blood partition coefficient. Note: QikProp predictions are for orally delivered drugs so, for example, dopamine and serotonin are CNS negative because they are too polar to cross the blood-brain barrier | –3.0 – 1.2 |
| **QPPMDCK** | Predicted apparent MDCK cell permeability in nm/sec. MDCK cells are considered to be a good mimic for the blood-brain barrier. QikProp predictions are for non-active transport. | <25 poor, >500 great |
| **QPlogKp** | Predicted skin permeability, log $K_p$. | –8.0 – –1.0 |
| **IP(ev)†** | PM3 calculated ionization potential (negative of HOMO energy). | 7.9 – 10.5 |
| **EA(eV)†** | PM3 calculated electron affinity (negative of LUMO energy). | –0.9 – 1.7 |
| **#metab‡** | Number of likely metabolic reactions. See Appendix A of the *QikProp User Manual* for a complete list of reactions. | 1 – 8 |
| **QPlogKhsa** | Prediction of binding to human serum albumin. | –1.5 – 1.5 |
| **HumanOralAbsorption** | Predicted qualitative human oral absorption: 1, 2, or 3 for low, medium, or high. The text version is reported in the output. The assessment uses a knowledge-based set of rules, including checking for suitable values of PercentHumanOralAbsorption, number of metabolites, number of rotatable bonds, logP, solubility and cell permeability. | |
| **PercentHumanOralAbsorption** | Predicted human oral absorption on 0 to 100% scale.The prediction is based on a quantitative multiple linear regression model. This property usually correlates well with HumanOralAbsorption, as both measure the same property. | >80% is high <25% is poor |
| **SAFluorine** | Solvent-accessible surface area of fluorine atoms. | 0.0 – 100.0 |
| **SAamideO** | Solvent-accessible surface area of amide oxygen atoms. | 0.0 – 35.0 |
| **PSA** | Van der Waals surface area of polar nitrogen and oxygen atoms and carbonyl carbon atoms. | 7.0 – 200.0 |
| **#NandO** | Number of nitrogen and oxygen atoms. | 2 – 15 |

*Table 2.1. QikProp properties and descriptors. Range is for 95% of known drugs. (Continued)*

| Property or Descriptor | Description | Range or recommended values |
|---|---|---|
| **RuleOfFive** | Number of violations of Lipinski's rule of five. The rules are: mol_MW < 500, QPlogPo/w < 5, donorHB ≤ 5, accptHB ≤ 10. Compunds that satisfy these rules are considered drug-like. (The "five" refers to the limits, which are multiples of 5.) | maximum is 4 |
| **RuleOfThree** | Number of violations of Jorgensen's rule of three. The three rules are: , QPlogS > -5.7, QP PCaco > 22 nm/s, # Primary Metabolites < 7. Compounds with fewer (and preferably no) violations of these rules are more likely to be orally available. | maximum is 3 |
| **#ringatoms** | Number of atoms in rings. | |
| **#in34** | Number of atoms in 3- or 4-membered rings. | |
| **#in56** | Number of atoms in 5- or 6-membered rings. | |
| **#noncon** | number of ring atoms not able to form conjugated aromatic systems (e.g. $sp^3$ C). | |
| **#nonHatm** | Number of heavy atoms (nonhydrogen atoms). | |
| **Jm** | Predicted maximum transdermal transport rate, $K_p \times MW \times S$ (μg $cm^{-2}$ $hr^{-1}$). $K_p$ and S are obtained from the aqueous solubility and skin permeability, QPlogKp and QPlogS. This property is only written to the output file: it is not used in any other calculations. | |